Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:45 AM EDT

PDB ID	:	1WU7
Title	:	Crystal structure of histidyl-tRNA synthetase from Thermoplasma acidophilum
Authors	:	Tanaka, Y.; Sakai, N.; Yao, M.; Watanabe, N.; Tamura, T.; Tanaka, I.
Deposited on	:	2004-12-01
Resolution	:	2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

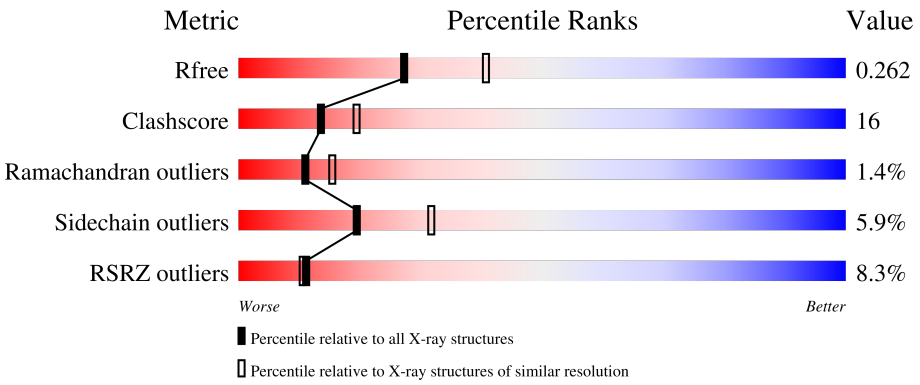
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	7% 67% 27% • •
1	B	434	8% 68% 25% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6955 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	424	3371	2123	586	647	2	13	0	0	0
1	B	420	3340	2104	579	642	2	13	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	20	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	175	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	214	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	228	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	242	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	300	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	312	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	348	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	360	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	367	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	404	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
A	427	LEU	-	EXPRESSION TAG	UNP Q9HLX5
A	428	GLU	-	EXPRESSION TAG	UNP Q9HLX5
A	429	HIS	-	EXPRESSION TAG	UNP Q9HLX5
A	430	HIS	-	EXPRESSION TAG	UNP Q9HLX5
A	431	HIS	-	EXPRESSION TAG	UNP Q9HLX5
A	432	HIS	-	EXPRESSION TAG	UNP Q9HLX5
A	433	HIS	-	EXPRESSION TAG	UNP Q9HLX5
A	434	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	20	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	175	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	214	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	228	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	242	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	300	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	312	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	348	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	360	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	367	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	404	MSE	MET	MODIFIED RESIDUE	UNP Q9HLX5
B	427	LEU	-	EXPRESSION TAG	UNP Q9HLX5
B	428	GLU	-	EXPRESSION TAG	UNP Q9HLX5
B	429	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	430	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	431	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	432	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	433	HIS	-	EXPRESSION TAG	UNP Q9HLX5
B	434	HIS	-	EXPRESSION TAG	UNP Q9HLX5

- Molecule 2 is water.

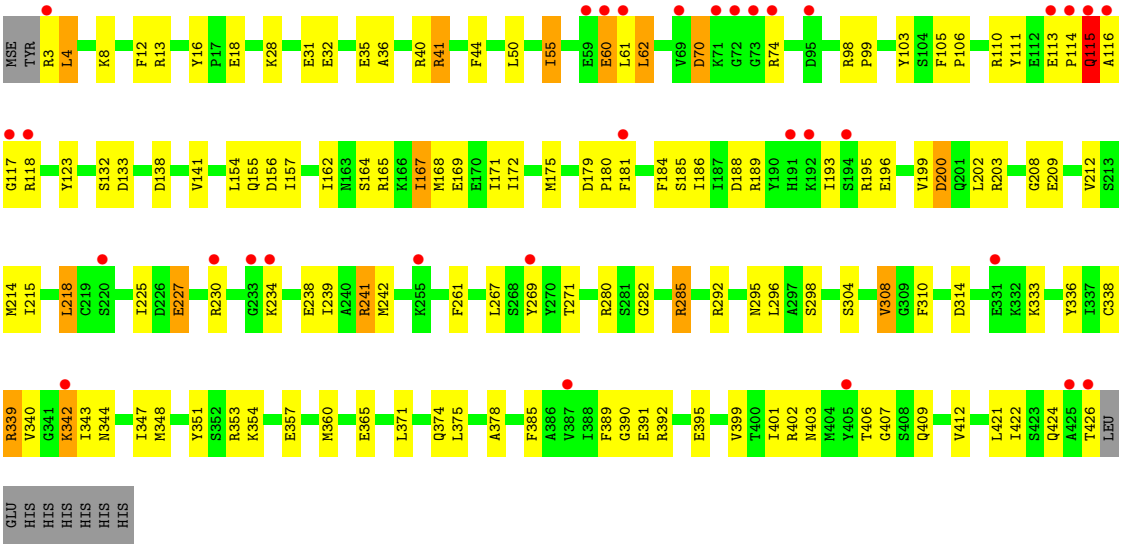
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	111	111	111	0	0
			Total	O		
2	B	133	133	133	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

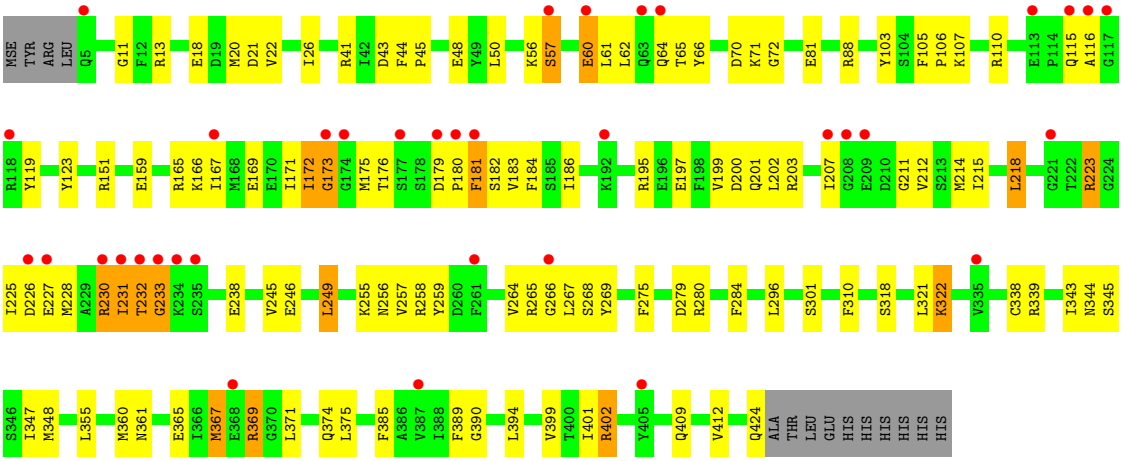
• Molecule 1: Histidyl-tRNA synthetase

Chain A:



• Molecule 1: Histidyl-tRNA synthetase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.70Å 101.73Å 167.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 19.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.40) 100.0 (19.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	15.29 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.263 0.210 , 0.262	Depositor DCC
R_{free} test set	4108 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6955	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.34	0/3415	0.59	0/4572
1	B	0.34	0/3384	0.59	0/4530
All	All	0.34	0/6799	0.59	0/9102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3371	0	3340	112	0
1	B	3340	0	3304	114	0
2	A	111	0	0	5	0
2	B	133	0	0	3	0
All	All	6955	0	6644	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:MSE:HE1	1:A:215:ILE:HD11	1.35	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:HB2	1:A:285:ARG:HH11	1.23	0.99
1:B:202:LEU:HG	1:B:207:ILE:HD12	1.52	0.88
1:A:4:LEU:HD12	1:A:4:LEU:H	1.39	0.86
1:B:197:GLU:HG2	1:B:201:GLN:HE21	1.43	0.83
1:A:41:ARG:HG3	1:A:41:ARG:HH11	1.47	0.77
1:B:225:ILE:HG22	1:B:259:TYR:HB2	1.68	0.75
1:A:70:ASP:HB3	1:A:74:ARG:O	1.88	0.74
1:A:292:ARG:HB2	1:A:308:VAL:HG13	1.70	0.73
1:B:159:GLU:OE2	1:B:258:ARG:NE	2.20	0.72
1:B:367:MSE:HE2	1:B:367:MSE:HA	1.74	0.70
1:A:343:ILE:HD13	1:A:389:PHE:HB3	1.74	0.69
1:B:343:ILE:HD13	1:B:389:PHE:HB3	1.75	0.69
1:B:56:LYS:O	1:B:57:SER:HB2	1.93	0.68
1:A:285:ARG:HH11	1:A:285:ARG:CB	2.02	0.68
1:B:385:PHE:HZ	1:B:424:GLN:HG3	1.60	0.67
1:A:344:ASN:O	1:A:347:ILE:HG22	1.94	0.67
1:A:203:ARG:HD3	1:A:209:GLU:OE2	1.93	0.67
1:A:402:ARG:HH21	1:A:407:GLY:HA2	1.58	0.66
1:A:31:GLU:O	1:A:35:GLU:HG3	1.94	0.66
1:B:179:ASP:C	1:B:181:PHE:H	1.98	0.66
1:A:375:LEU:HD13	1:A:402:ARG:HH11	1.61	0.66
1:B:339:ARG:CZ	1:B:348:MSE:HE1	2.26	0.66
1:B:175:MSE:HG3	1:B:176:THR:H	1.59	0.66
1:B:264:VAL:O	1:B:265:ARG:HB2	1.97	0.65
1:B:345:SER:HA	1:B:348:MSE:HE3	1.78	0.64
1:B:267:LEU:HD23	1:B:269:TYR:OH	1.98	0.64
1:A:132:SER:O	1:A:292:ARG:NH2	2.30	0.64
1:B:345:SER:HA	1:B:348:MSE:CE	2.29	0.63
1:A:186:ILE:HG21	1:A:202:LEU:HD22	1.81	0.63
1:B:62:LEU:HD12	1:B:65:THR:HG21	1.80	0.63
1:B:225:ILE:HG13	1:B:226:ASP:N	2.12	0.63
1:B:11:GLY:O	1:B:119:TYR:HB3	1.98	0.63
1:A:164:SER:HB3	1:A:167:ILE:HB	1.80	0.63
1:A:40:ARG:HD3	2:A:568:HOH:O	1.97	0.62
1:B:202:LEU:HD21	1:B:215:ILE:HG21	1.81	0.62
1:B:267:LEU:HD23	1:B:269:TYR:CZ	2.35	0.62
1:A:99:PRO:HD3	1:B:367:MSE:CG	2.29	0.62
1:A:269:TYR:OH	1:A:296:LEU:HD22	1.99	0.62
1:A:165:ARG:O	1:A:169:GLU:HG3	2.00	0.62
1:A:227:GLU:O	1:A:230:ARG:HG2	2.00	0.60
1:B:48:GLU:CD	1:B:88:ARG:HH22	2.05	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ARG:NH2	1:B:280:ARG:HH22	1.99	0.60
1:B:394:LEU:HD13	1:B:394:LEU:O	2.02	0.59
1:B:56:LYS:O	1:B:57:SER:CB	2.51	0.59
1:B:179:ASP:O	1:B:181:PHE:N	2.34	0.59
1:A:141:VAL:HG13	1:A:310:PHE:HD2	1.68	0.58
1:B:60:GLU:HG2	1:B:266:GLY:O	2.03	0.58
1:A:138:ASP:OD1	1:A:292:ARG:NH1	2.36	0.58
1:B:365:GLU:OE1	1:B:369:ARG:HD2	2.03	0.57
1:A:16:TYR:HB3	1:A:18:GLU:OE2	2.05	0.57
1:B:195:ARG:O	1:B:199:VAL:HG23	2.05	0.57
1:B:197:GLU:CG	1:B:201:GLN:HE21	2.16	0.57
1:A:167:ILE:HG13	1:A:242:MSE:CE	2.35	0.56
1:B:18:GLU:CD	1:B:18:GLU:H	2.09	0.56
1:B:228:MSE:SE	1:B:231:ILE:HD11	2.55	0.56
1:A:116:ALA:O	1:A:118:ARG:N	2.38	0.56
1:A:168:MSE:HB3	1:A:184:PHE:CE1	2.41	0.56
1:A:203:ARG:HG2	1:A:212:VAL:HG21	1.88	0.56
1:A:155:GLN:O	1:A:156:ASP:HB2	2.06	0.55
1:B:165:ARG:O	1:B:169:GLU:HB3	2.06	0.55
1:A:98:ARG:HG3	1:A:99:PRO:HA	1.89	0.55
1:A:13:ARG:O	1:B:45:PRO:HD3	2.07	0.55
1:A:402:ARG:HB3	1:A:409:GLN:HB3	1.89	0.54
1:A:195:ARG:O	1:A:199:VAL:HG23	2.08	0.54
1:A:339:ARG:HD2	1:A:348:MSE:HE1	1.88	0.54
1:B:48:GLU:OE1	1:B:88:ARG:NH2	2.35	0.54
1:A:36:ALA:HA	1:B:361:ASN:HD22	1.73	0.54
1:B:401:ILE:HD12	1:B:412:VAL:HG21	1.89	0.54
1:A:99:PRO:HD3	1:B:367:MSE:HG3	1.90	0.53
1:B:183:VAL:HB	1:B:186:ILE:HD12	1.91	0.53
1:B:175:MSE:SE	1:B:214:MSE:HE2	2.59	0.53
1:A:18:GLU:H	1:A:18:GLU:CD	2.12	0.52
1:A:113:GLU:C	1:A:115:GLN:H	2.13	0.52
1:B:258:ARG:HH21	1:B:280:ARG:HH22	1.58	0.52
1:B:175:MSE:HG3	1:B:176:THR:N	2.24	0.52
1:B:200:ASP:HA	1:B:203:ARG:HB3	1.92	0.52
1:A:343:ILE:HD12	1:A:389:PHE:O	2.10	0.51
1:B:186:ILE:HD13	1:B:202:LEU:HA	1.92	0.51
1:B:230:ARG:HD3	1:B:231:ILE:HG23	1.92	0.51
1:B:182:SER:C	1:B:184:PHE:H	2.12	0.51
1:B:186:ILE:HG21	1:B:202:LEU:HD13	1.93	0.51
1:A:351:TYR:HA	1:A:354:LYS:NZ	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HD11	1:A:239:ILE:HG12	1.91	0.50
1:A:123:TYR:OH	1:B:43:ASP:OD2	2.23	0.50
1:A:133:ASP:HA	1:A:292:ARG:NH2	2.27	0.50
1:B:171:ILE:C	1:B:173:GLY:H	2.15	0.50
1:A:168:MSE:O	1:A:172:ILE:HG12	2.11	0.50
1:A:401:ILE:HD12	1:A:412:VAL:HG21	1.94	0.50
1:B:57:SER:HA	1:B:268:SER:OG	2.12	0.50
1:A:55:ILE:HG12	2:A:544:HOH:O	2.10	0.50
1:A:61:LEU:HD13	1:A:61:LEU:O	2.12	0.50
1:A:167:ILE:HG12	1:A:238:GLU:HG3	1.93	0.50
1:A:8:LYS:HB3	1:B:88:ARG:NH1	2.27	0.49
1:A:343:ILE:HD11	1:A:390:GLY:C	2.32	0.49
1:A:336:TYR:CD1	1:A:378:ALA:HB2	2.47	0.49
1:B:367:MSE:HA	1:B:367:MSE:CE	2.41	0.49
1:B:375:LEU:HD13	1:B:402:ARG:HH21	1.77	0.49
1:A:40:ARG:NH2	1:B:21:ASP:OD2	2.46	0.49
1:B:402:ARG:HB2	1:B:409:GLN:HG2	1.95	0.49
1:A:353:ARG:O	1:A:357:GLU:HG3	2.13	0.49
1:B:61:LEU:HD21	1:B:110:ARG:NH1	2.27	0.48
1:B:179:ASP:C	1:B:181:PHE:N	2.64	0.48
1:A:339:ARG:HD2	1:A:348:MSE:CE	2.43	0.48
1:A:4:LEU:HD12	1:A:4:LEU:N	2.19	0.48
1:A:113:GLU:O	1:A:115:GLN:N	2.47	0.48
1:B:64:GLN:HG3	1:B:110:ARG:HB3	1.96	0.48
1:A:336:TYR:OH	1:A:365:GLU:OE2	2.31	0.48
1:B:231:ILE:O	1:B:232:THR:HB	2.14	0.48
1:B:225:ILE:O	1:B:228:MSE:HB2	2.13	0.48
1:B:367:MSE:HB2	1:B:369:ARG:HG2	1.94	0.48
1:A:360:MSE:HE2	1:A:422:ILE:HG12	1.94	0.48
1:A:41:ARG:HG3	1:A:41:ARG:NH1	2.23	0.47
1:B:172:ILE:HG13	1:B:172:ILE:O	2.13	0.47
1:B:355:LEU:HD22	1:B:360:MSE:HE1	1.96	0.47
1:B:218:LEU:HD11	1:B:231:ILE:HD12	1.96	0.47
1:A:154:LEU:O	1:A:157:ILE:HG12	2.15	0.47
1:B:424:GLN:O	1:B:424:GLN:HG2	2.15	0.47
1:B:318:SER:O	1:B:322:LYS:HE3	2.15	0.47
1:B:70:ASP:OD1	1:B:72:GLY:N	2.45	0.47
1:A:111:TYR:CD2	1:B:71:LYS:NZ	2.82	0.47
1:A:234:LYS:HD2	2:A:563:HOH:O	2.13	0.47
1:A:338:CYS:HB2	1:A:374:GLN:NE2	2.29	0.47
1:A:371:LEU:HD13	1:A:371:LEU:C	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ILE:O	1:A:175:MSE:HG3	2.14	0.47
1:B:71:LYS:NZ	1:B:71:LYS:HB2	2.30	0.46
1:B:344:ASN:HB3	2:B:553:HOH:O	2.15	0.46
1:B:245:VAL:O	1:B:249:LEU:HD22	2.14	0.46
1:A:167:ILE:HG22	1:A:168:MSE:N	2.31	0.46
1:A:403:ASN:HD21	1:A:426:THR:HA	1.79	0.46
1:B:50:LEU:HD11	1:B:62:LEU:HD11	1.95	0.46
1:B:180:PRO:O	1:B:182:SER:N	2.48	0.46
1:B:199:VAL:HG13	1:B:212:VAL:HG11	1.98	0.46
1:A:271:THR:HG21	1:A:295:ASN:ND2	2.30	0.46
1:B:107:LYS:HE3	1:B:123:TYR:OH	2.16	0.46
1:A:375:LEU:HD13	1:A:402:ARG:NH1	2.30	0.46
1:A:402:ARG:CB	1:A:409:GLN:HB3	2.45	0.46
1:A:115:GLN:HG3	2:A:640:HOH:O	2.15	0.45
1:A:3:ARG:HB3	1:B:301:SER:C	2.37	0.45
1:A:339:ARG:HD2	1:A:348:MSE:SE	2.66	0.45
1:A:340:VAL:HG13	1:A:340:VAL:O	2.16	0.45
1:B:279:ASP:HB3	1:B:284:PHE:O	2.16	0.45
1:B:344:ASN:O	1:B:347:ILE:HG22	2.16	0.45
1:B:13:ARG:HD3	1:B:119:TYR:CE1	2.51	0.45
1:B:231:ILE:HG13	1:B:232:THR:HG22	1.99	0.45
1:A:50:LEU:HD11	1:A:62:LEU:HG	1.99	0.45
1:A:179:ASP:HA	1:A:180:PRO:HD3	1.85	0.45
1:A:342:LYS:H	1:A:342:LYS:HD2	1.82	0.45
1:B:61:LEU:CD1	1:B:81:GLU:HB3	2.47	0.45
1:B:256:ASN:HB3	1:B:258:ARG:HH22	1.82	0.45
1:A:167:ILE:HG13	1:A:242:MSE:HE1	1.99	0.44
1:B:22:VAL:O	1:B:26:ILE:HG13	2.17	0.44
1:B:175:MSE:HG3	1:B:176:THR:HG22	1.99	0.44
1:A:185:SER:O	1:A:188:ASP:HB3	2.18	0.44
1:A:214:MSE:HG2	1:A:218:LEU:HD22	2.00	0.44
1:B:355:LEU:HD22	1:B:360:MSE:CE	2.48	0.44
1:A:189:ARG:O	1:A:193:ILE:HG12	2.18	0.44
1:B:41:ARG:HB2	1:B:103:TYR:CZ	2.53	0.44
1:A:343:ILE:HD11	1:A:391:GLU:N	2.33	0.44
1:A:392:ARG:HA	1:A:395:GLU:OE2	2.17	0.44
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.32	0.44
1:B:225:ILE:HD13	1:B:246:GLU:CD	2.38	0.44
1:A:41:ARG:HG2	1:B:20:MSE:HE2	1.99	0.44
1:A:36:ALA:HA	1:B:361:ASN:ND2	2.33	0.43
1:A:181:PHE:HA	1:A:184:PHE:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:O	1:A:200:ASP:OD1	2.36	0.43
1:B:375:LEU:HD13	1:B:402:ARG:NH2	2.33	0.43
1:B:211:GLY:O	1:B:215:ILE:HG13	2.18	0.43
1:A:28:LYS:O	1:A:32:GLU:HG3	2.19	0.43
1:B:184:PHE:N	1:B:184:PHE:CD1	2.87	0.43
1:A:333:LYS:NZ	1:A:421:LEU:O	2.49	0.43
1:B:166:LYS:HB2	1:B:238:GLU:HG2	2.00	0.43
1:A:3:ARG:HB3	1:B:301:SER:O	2.18	0.43
1:A:167:ILE:HD11	1:A:239:ILE:CG1	2.48	0.43
1:A:280:ARG:C	1:A:282:GLY:H	2.21	0.43
1:B:62:LEU:HA	1:B:65:THR:HG23	2.00	0.42
1:A:403:ASN:HB3	1:A:406:THR:OG1	2.19	0.42
1:B:167:ILE:HG13	1:B:238:GLU:CG	2.49	0.42
1:B:343:ILE:HD11	1:B:390:GLY:C	2.40	0.42
1:A:230:ARG:HG3	1:A:230:ARG:HH11	1.85	0.42
1:B:176:THR:O	1:B:176:THR:HG23	2.19	0.42
1:A:162:ILE:HD11	1:A:225:ILE:HD11	2.02	0.42
1:A:351:TYR:HA	1:A:354:LYS:HZ3	1.83	0.42
1:B:338:CYS:HB3	1:B:374:GLN:OE1	2.20	0.42
1:A:113:GLU:OE1	1:A:113:GLU:HA	2.20	0.42
1:A:402:ARG:HH21	1:A:407:GLY:CA	2.28	0.42
1:A:298:SER:OG	1:A:304:SER:HA	2.20	0.41
1:A:385:PHE:CZ	1:A:426:THR:HG23	2.55	0.41
1:B:184:PHE:N	1:B:184:PHE:HD1	2.18	0.41
1:A:241:ARG:HG2	1:A:241:ARG:HH11	1.86	0.41
1:B:245:VAL:HG12	1:B:249:LEU:CD2	2.50	0.41
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.87	0.41
1:B:233:GLY:N	2:B:683:HOH:O	2.53	0.41
1:B:275:PHE:CZ	1:B:310:PHE:HB3	2.56	0.41
1:B:151:ARG:CZ	2:B:637:HOH:O	2.68	0.41
1:A:195:ARG:NH1	1:A:195:ARG:HG3	2.35	0.41
1:A:199:VAL:HG12	1:A:203:ARG:NE	2.36	0.41
1:B:230:ARG:HD3	1:B:231:ILE:N	2.36	0.41
1:A:60:GLU:CD	1:A:61:LEU:H	2.24	0.41
1:A:195:ARG:HG3	1:A:195:ARG:HH11	1.86	0.41
1:B:197:GLU:O	1:B:201:GLN:HG3	2.21	0.41
1:A:31:GLU:HG2	1:A:103:TYR:OH	2.20	0.41
1:A:98:ARG:HD3	2:A:601:HOH:O	2.19	0.41
1:B:255:LYS:O	1:B:256:ASN:HB2	2.21	0.41
1:A:12:PHE:HB3	1:B:45:PRO:HB3	2.03	0.41
1:A:155:GLN:O	1:A:156:ASP:CB	2.66	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:CD1	1:B:202:LEU:HD12	2.51	0.40
1:B:256:ASN:O	1:B:258:ARG:CZ	2.69	0.40
1:A:208:GLY:O	1:A:212:VAL:HG23	2.22	0.40
1:A:292:ARG:CZ	1:A:308:VAL:HG22	2.51	0.40
1:B:227:GLU:O	1:B:231:ILE:HG12	2.21	0.40
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.91	0.40
1:A:168:MSE:SE	1:A:261:PHE:CE1	3.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	422/434 (97%)	403 (96%)	15 (4%)	4 (1%)	17 25
1	B	418/434 (96%)	390 (93%)	20 (5%)	8 (2%)	8 10
All	All	840/868 (97%)	793 (94%)	35 (4%)	12 (1%)	11 15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	GLY
1	B	181	PHE
1	B	233	GLY
1	A	114	PRO
1	A	115	GLN
1	B	57	SER
1	B	116	ALA
1	A	227	GLU
1	B	172	ILE
1	B	232	THR
1	B	173	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	231	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/356 (101%)	337 (94%)	23 (6%)	17	28
1	B	357/356 (100%)	338 (95%)	19 (5%)	22	37
All	All	717/712 (101%)	675 (94%)	42 (6%)	19	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	41	ARG
1	A	44	PHE
1	A	55	ILE
1	A	60	GLU
1	A	62	LEU
1	A	70	ASP
1	A	105	PHE
1	A	106	PRO
1	A	110	ARG
1	A	115	GLN
1	A	167	ILE
1	A	200	ASP
1	A	218	LEU
1	A	241	ARG
1	A	267	LEU
1	A	285	ARG
1	A	308	VAL
1	A	314	ASP
1	A	339	ARG
1	A	342	LYS
1	A	399	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	424	GLN
1	B	44	PHE
1	B	60	GLU
1	B	66	TYR
1	B	105	PHE
1	B	106	PRO
1	B	115	GLN
1	B	218	LEU
1	B	223	ARG
1	B	230	ARG
1	B	249	LEU
1	B	257	VAL
1	B	296	LEU
1	B	321	LEU
1	B	322	LYS
1	B	367	MSE
1	B	369	ARG
1	B	371	LEU
1	B	399	VAL
1	B	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	97	GLN
1	A	295	ASN
1	A	344	ASN
1	A	374	GLN
1	A	424	GLN
1	B	63	GLN
1	B	64	GLN
1	B	122	HIS
1	B	201	GLN
1	B	295	ASN
1	B	361	ASN
1	B	409	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/434 (94%)	0.21	32 (7%)	13	11	19, 40, 73, 90	0
1	B	407/434 (93%)	0.23	36 (8%)	10	9	16, 39, 85, 101	0
All	All	818/868 (94%)	0.22	68 (8%)	11	10	16, 40, 79, 101	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	TYR	7.5
1	B	179	ASP	6.6
1	A	405	TYR	6.3
1	B	174	GLY	5.8
1	B	180	PRO	5.6
1	A	115	GLN	5.6
1	B	235	SER	5.5
1	A	3	ARG	5.3
1	A	116	ALA	5.3
1	B	116	ALA	5.3
1	B	117	GLY	5.2
1	B	230	ARG	5.0
1	B	233	GLY	4.9
1	B	231	ILE	4.6
1	A	73	GLY	4.6
1	A	331	GLU	4.3
1	B	232	THR	4.3
1	A	72	GLY	4.3
1	A	117	GLY	4.3
1	A	426	THR	4.2
1	A	74	ARG	4.2
1	B	181	PHE	4.1
1	A	234	LYS	4.0
1	B	209	GLU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	230	ARG	3.9
1	A	61	LEU	3.8
1	B	234	LYS	3.8
1	A	342	LYS	3.8
1	B	368	GLU	3.6
1	A	59	GLU	3.4
1	A	192	LYS	3.4
1	B	118	ARG	3.4
1	A	71	LYS	3.4
1	A	60	GLU	3.3
1	A	233	GLY	3.3
1	B	115	GLN	3.3
1	B	226	ASP	3.0
1	A	181	PHE	3.0
1	B	227	GLU	2.9
1	A	425	ALA	2.8
1	A	191	HIS	2.7
1	A	113	GLU	2.7
1	B	208	GLY	2.6
1	A	114	PRO	2.6
1	B	57	SER	2.6
1	B	192	LYS	2.6
1	B	221	GLY	2.5
1	B	266	GLY	2.5
1	B	387	VAL	2.4
1	B	177	SER	2.4
1	B	167	ILE	2.4
1	B	173	GLY	2.4
1	B	113	GLU	2.4
1	A	269	TYR	2.3
1	B	63	GLN	2.3
1	A	69	VAL	2.3
1	B	64	GLN	2.3
1	B	261	PHE	2.2
1	B	335	VAL	2.2
1	B	207	ILE	2.2
1	A	387	VAL	2.2
1	A	95	ASP	2.1
1	A	118	ARG	2.1
1	A	194	SER	2.1
1	B	5	GLN	2.1
1	A	255	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	220	SER	2.1
1	B	60	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.